International Journal of Physics
and Research (IJPR)
ISSN (P): 2250–0030; ISSN (E): 2319–4499
Vol. 9, Issue 2, Dec 2019, 1–6

SPECIES DENSITIES OF DIELECTRIC BARRIER DISCHARGE (DBD) NON-THERMAL NITROGEN PLASMA

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ABSTRACT

Species densities of Nitrogen plasma are investigated using MATLAB simulation technique. In this simulation, a total of nine reactions with known reaction rate coefficients are used. From these reactions we get continuity equations which are simulated based on the steady state rate balance equations (non-linear equations) derived from the continuity equations. The whole simulation is performed on MATLAB application software using f solve function. Then the species densities at temperature 300 K by the f solve values are determined. Electron density has been estimated from this simulation and is in the order 10^{18} cm^{-3}. The densities of different Reactive Nitrogen Species are determined from pressure 1 torr to 760 torr are tabulated and discussed.

KEYWORDS: Species Density, MATHLAB Simulation, Nitrogen & Plasma

Received: Jun 03, 2019; **Accepted:** Jun 23, 2019; **Published:** Aug 16, 2019; **Paper Id.:** IJPRDEC20191

Original Article

1. INTRODUCTION

Plasma is a quasi neutral ionized gas roughly equal number of positive (ions) and negative (electrons) ions. Like gas, it have no fixed shape or volume and less dense then solid or liquid. Unlike gas, it has equal number of ions of opposite charge. Plasma can be found in two ways, naturally produced plasma in sun, in various stars or in our earth's atmosphere and plasma created in the laboratory. Various methods can be used to produce plasma in laboratory but one of the most effective and efficient way is by dielectric barrier discharge (DBD). Di electric barrier discharge (DBD) is a kind of gas discharge developed in 1857 by Werner von Siemens as a process for Ozone production. For its irrelatively low cost, low operation temperature and of high pressure it has numerous numbers of applications like de-pollution of a confined place, biological applications and material surface processing applications. It is proved that DBD can be an effective source of different reactive species such as O_3, NO, N, O, OH etc. N (4S), N+ and free electrons are the main species with energy conservation non-equilibrium excitation in the post-discharge period [1]. In the inelastic collision there energy and momentum is not the same as it was before collisions. Energy transferred from one species to another during the collisions between various species creates excitations. This collision sometime generates new species. The generation of new species mainly depends on the kinetics of the various species. In the real world it's hard to generate a specific species of plasma. Before generation of specific plasma, simulation is to be performing under various conditions. This simulation is time and cost efficient. In addition it also gives us the idea of instrument it required. Simulation can be modelled on various ways. Kinetic modelling helps to simulate a system that contains various elements (such as gas, radicals, ions, electron etc.). Kinetic model is based on the kinetics of the elements in plasma. In this paper a simulation based on some reaction in Nitrogen plasma is performed in a close system at 300 K to get different species densities.

2. PLASMA MODELLING

During different applications of plasma, the plasma properties can be divided into the following subgroups like physical processes, gas phase kinetics and surface interactions [2]. For simulations a particular plasma process needs to deal with the above processes. Depending upon the methods of simulation on theoretical approach we see different types of simulation techniques like MATHLAB f solve, Monti-Carlo Simulation etc. For determining the plasma properties Numerical Modelling is computer based method. For structural and fluid investigation this method is useful by the application of laws of mechanics depending on the number of pre-prepared code which can be used for linear of non-linear analysis. In order to reproduce the plasma properties using the effect of mechanics and to predict the reaction of various plasma variables numerical modelling is a useful tool. Numerical models are also a useful tool for modelling plasma systems that are too complex for analytical modelling methods to be used [3, 4].

2.1 Kinetic Modelling

To describe plasma, the kinetic model is a fundamental way, which produce a distribution function$f(\vec{x},\vec{v},t)$, where the independent variables $\vec{x}$and $\vec{v}$ are position and velocity, respectively [5]. By solving the Boltzmann equation, a kinetic description is achieved. When the description of long-range Coulomb interaction is needed, by the V solve equation which contains self-consistent collective electromagnetic field, or by Fokker-Plank equation, where approximation have been used to drive manageable collision terms. Using Maxwell's equations the charges and currents produced by the self-consistent distribution functions can be determined.

We get the species velocity distribution functions from the solution variables in the kinetic models. It is assumed for fluid models that the distribution function is in equilibrium. Then the Boltzmann equation can be replaced by its corresponding conservation of mass, momentum and energy [6].

The plasma modelling in a continuum regime starts from the Boltzmann equations [6]

$$\frac{\partial f_i}{\partial t} + c_i.\nabla f_i + \mathbf{F}.\nabla_c\left(\frac{f_i}{m_i}\right) = \left(\frac{\partial f_i}{\partial t}\right)_{coll} \quad (1)$$

Where the index i, f, c, F, ∇ and ∇_cindicate single species, distribution function, the charged particle velocity, the force, the gradient operator in physical space and the gradient operator in velocity space.

The subscript '*coll.*' refers the change of velocity distribution due to collision. F represents the Lorentz force on the charged particles. A detailed discussion on the theory of Boltzmann equation and its relation for the fluid models is presented in [6, 7]. The index 'i' indicate for every type of species. To get self-consistent solution of the above we need to solve for the electric field E by means of Poisson's equation

$$\nabla.\boldsymbol{E} = \frac{\rho}{\varepsilon_0} \quad (2)$$

2.2 Reaction and Rate Balance Equations

The considered Nitrogen plasma reactions and there rate coefficients at 300 K are tabulated in table 1.

Table 1: Reaction & Rate Coefficient at 300 K

No.	Reaction	Reaction Rate, k	Reference
1	$N_2(A) + N_2(a') \rightarrow N_4^+ + e$	4.0×10^{-12}	[8,1]
2	$N_2(a') + N_2(a') \rightarrow N_4^+ + e$	1.0×10^{-11}	[8,1]

Table 1: Contd.,			
3	$N_2^+ + N_2(A) \rightarrow N_3^+ + N$	3.0×10^{-10}	[9,1]
4	$N_3^+ + N \rightarrow N_2^+ + N_2$	6.6×10^{-11}	[8]
5	$N_2(A) + N \rightarrow N_2 + N$	2×10^{-12}	[8,1]
6	$N_2(A) + N \rightarrow N_2 + N(\,^2P)$	4×10^{-11}	[8,1]
7	$N_2(A) + N_2 \rightarrow 2N_2$	3.0×10^{-16}	[8,1]
8	$N_2^+ + N \rightarrow N^+ + N_2$	7.2×10^{-13}	[10]
9	$N(\,^2P) + N_2 \rightarrow N_2 + N$	6×10^{-14}	[10,13]

All the reactions are considered in the closed system having at temperature 300 K. The reactions are assembled into a model for intrinsic chemical kinetics for the concentration of these ten species [11]. If the reactor is assumed kinetics dominated (well mixed)-when there action time is much shorter than the am bipolar diffusion time, then each of the elementary reactions in Table-1contributes mass action law terms to the kinetics model with rate constants, with number densities defined as: $N_{N_2}$is the density of N_2; $N_{N_2(A)}$the density of $N_2(A)$; $N_{N_2(a')}$the density of $N_2(a')$; $N_N$the density of N; $N_{N(\,^2P)}$the density of $N(\,^2P)$; $N_{N^+}$the density of N^+; $N_{N_2^+}$the density of N_2^+; $N_{N_3^+}$is the density of N_3^+; $N_{N_4^+}$the density of N_4^+ and N_e the density of electron [11].

The species density is a function of time. The continuity equation is needed to simulate the time dependent behaviour of the Nitrogen plasma species densities. Now we can write the continuity equations from the reactions and rate coefficients that shown in table 1 as

$$\frac{dN_{N_2}}{dt} = k_4 N_{N_2^+} N_{N_2} + k_5 N_{N_2} N_N + k_6 N_{N_2} N_{N(\,^2P)} - k_7 N_{N_2(A)} N_{N_2} + k_7 N_{N_2} N_{N_2} + k_8 N_{N^+} N_{N_2} - k_9 N_{N(\,^2P)} N_{N_2} + k_9 N_N N_{N_2} \quad (3)$$

$$\frac{dN_{N_2(A)}}{dt} = -k_1 N_{N_2(A)} N_{N_2(a')} - k_3 N_{N_2^+} N_{N_2(A)} - k_5 N_{N_2(A)} N_N - k_6 N_{N_2(A)} N_N - k_7 N_{N_2(A)} N_{N_2} \quad (4)$$

$$\frac{dN_{N_2(a')}}{dt} = -k_1 N_{N_2(A)} N_{N_2(a')} - k_2 N_{N_2(a')} N_{N_2(a')} \quad (5)$$

$$\frac{dN_N}{dt} = k_3 N_{N_3^+} N_N - k_4 N_{N_3^+} N_N - k_5 N_{N_2(A)} N_N + k_5 N_{N_2} N_N - k_6 N_{N_2(A)} N_N - k_8 N_{N_2^+} N_N + k_9 N_{N_2} N_N \quad (6)$$

$$\frac{dN_{N(\,^2P)}}{dt} = k_6 N_{N_2} N_{N(\,^2P)} - k_9 N_{N(\,^2P)} N_{N_2} \quad (7)$$

$$\frac{dN_{N^+}}{dt} = k_9 N_{N^+} N_{N_2} \quad (8)$$

$$\frac{dN_{N_2^+}}{dt} = -k_3 N_{N_2^+} N_{N_2(A)} + k_4 N_{N_2^+} N_{N_2} - k_8 N_{N_2^+} N_N \quad (9)$$

$$\frac{dN_{N_3^+}}{dt} = k_3 N_{N_3^+} N_N - k_4 N_{N_3^+} N_N \quad (10)$$

$$\frac{dN_{N_4^+}}{dt} = k_1 N_{N_4^+} N_e + k_2 N_{N_4^+} N_e \quad (11)$$

$$\frac{dN_e}{dt} = k_1 N_{N_4^+} N_e + k_2 N_{N_4^+} N_e \tag{12}$$

At first, simulation of Nitrogen plasma discharge is performed. Here the chemical kinetics is clearly simplified and Nitrogen is the main product [11]. By solving the steady state rate balance equations we calculate the species density to see the plasma composition on atmospheric pressure and at temperature 300 K.

To get the solution we need to deduce steady state balance equations from the differential equations in previous section. The steady state balance equations are derived as

$$k_4 N_{N_2^+} N_{N_2} + k_5 N_{N_2} N_N + k_6 N_{N_2} N_{N(\,^2P)} - k_7 N_{N_2(A)} N_{N_2} + k_7 N_{N_2} N_{N_2} + k_8 N_{N^+} N_{N_2} - k_9 N_{N(\,^2P)} N_{N_2} + k_9 N_N N_{N_2} = 0 \tag{13}$$

$$-k_1 N_{N_2(A)} N_{N_2(a')} - k_3 N_{N_2^+} N_{N_2(A)} - k_5 N_{N_2(A)} N_N - k_6 N_{N_2(A)} N_N - k_7 N_{N_2(A)} N_{N_2} = 0 \tag{14}$$

$$-k_1 N_{N_2(A)} N_{N_2(a')} - k_2 N_{N_2(a')} N_{N_2(a')} = 0 \tag{15}$$

$$k_3 N_{N_3^+} N_N - k_4 N_{N_3^+} N_N - k_5 N_{N_2(A)} N_N + k_5 N_{N_2} N_N - k_6 N_{N_2(A)} N_N - k_8 N_{N_2^+} N_N + k_9 N_{N_2} N_N = 0 \tag{16}$$

$$k_6 N_{N_2} N_{N(\,^2P)} - k_9 N_{N(\,^2P)} N_{N_2} = 0 \tag{17}$$

$$k_9 N_{N^+} N_{N_2} = 0 \tag{18}$$

$$-k_3 N_{N_2^+} N_{N_2(A)} + k_4 N_{N_2^+} N_{N_2} - k_8 N_{N_2^+} N_N = 0 \tag{19}$$

$$k_3 N_{N_3^+} N_N - k_4 N_{N_3^+} N_N = 0 \tag{20}$$

$$k_1 N_{N_4^+} N_e + k_2 N_{N_4^+} N_e = 0 \tag{21}$$

$$k_1 N_{N_4^+} N_e + k_2 N_{N_4^+} N_e = 0 \tag{22}$$

3. RESULTS

The Nitrogen plasma species densities from pressure 1 torr to atmospheric pressure (760 torr) at 300 K are shown in figure 1. All the species density for various pressures was determined [11] using the ideal gas law i. e. $PV = nRT$, where, P is the pressure of the gas, V is the volume of the gas,n is the amount of species in the gas mixture, R is the ideal, or universal, gas constant, equal to the product of the Boltzmann constant and the Avogadro constant and T is the absolute temperature of the gas [12]. From the result we see that at 1 torr the density of nitrogen is $2.278 \times 10^{16} cm^{-3}$and it increases with pressure and become maximum i. e.$1.731 \times 10^{19}\ cm^{-3}$ at atmospheric pressure. Metastable Nitrogen and atomic Nitrogen densities are $4.390 \times 10^{15}\ cm^{-3}$ and $1.723 \times 10^{15}\ cm^{-3}$at 1 torr and $3.336 \times 10^{18}\ cm^{-3}$ and $1.309 \times 10^{18}\ cm^{-3}$ at atmospheric pressure respectively. The electron density is $5.504 \times 10^{15} cm^{-3}$at 1 torr and $4.183 \times 10^{18}\ cm^{-3}$at atmospheric pressure. From the figure 1, it is observed that species density increase rapidly at 1 torr to 50 torr. After 50 torr it increases slowly.

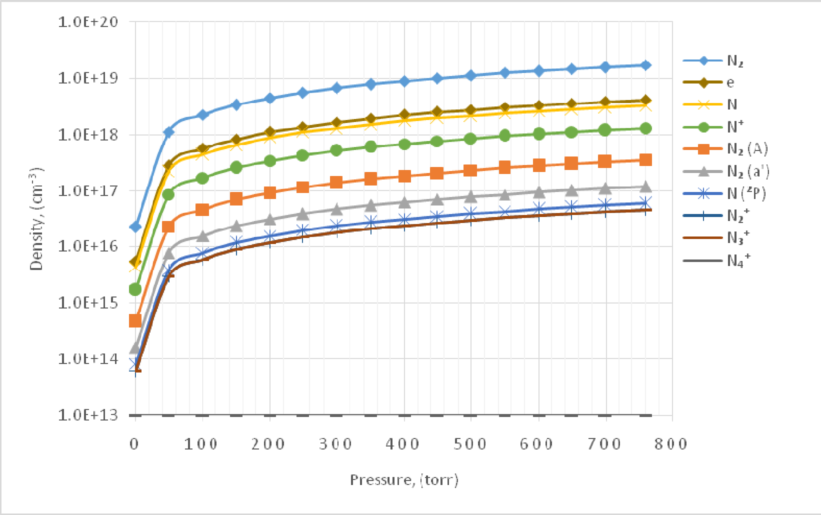

Figure 1: Species Density Vs Pressure Curve of Nitrogen plasma at 300 K

4. CONCLUSIONS

We performed a mathematical simulation on the Nitrogen plasma discharge to find the species for various pressures at temperature $300\ K$. The species density of various Nitrogen plasma species are calculated from the MATLAB simulation. From the result we see that in the plasma discharge there are neutral nitrogen, atomic nitrogen, ionized nitrogen and free electron. The electron density is of the order of $10^{15} cm^{-3}$ at 1 torr and$10^{18} cm^{-3}$at atmospheric pressure and at 300 K. From the figure 1 we see that species density increase rapidly at 1 torr to 50 torr. After 50 torr it increases slowly. It is observed that a significant amount of Reactive Nitrogen Species (RNS) is produced in the Nitrogen plasma which can be used for different applications.

REFERENCES

1. *Tsyganov, Dmitry; Pancheshnyi, Sergey, Simulation of N-atom production in dielectric-barrier discharge in nitrogen at atmospheric pressure, Plasma Sources Sci. Technol.* ***21*** *065010 (2012).*
2. *www.plasmatech.gr [Internet source].*
3. *https://openei.org/wiki/Numerical-Modeling.*
4. *http://hyperphysics.phy-astr.gsu.edu/hbase/elacol.html.*
5. *en.wikipedia.org [Internet source].*
6. *Jayaraman Balaji, Shyy Wei, "Modeling of dielectric barrier discharge-induced fluid dynamics and heat transfer", Progress in Aerospace Sciences, Volume 44, Issue 3, 2008, p. 139–191.*
7. *E. Gogolides and H. H. Sawin, "Continuum modeling of radio-frequency glow discharges. I. Theory and results for electropositive and electronegative gases," J. Appl. Phys.* ***72(9)****, pp 3971–3987 (1992).*
8. *Geete, A., & Khandwawala, A. I. (2014). Exergy analysis for 120MW thermal power plant with different inlet temperature conditions. International Journal of Research in Engineering & Technology, 2(1), 21–30.*
9. *Capitelli M, Ferreira C M, Gordiets B F and Osipov A I, Plasma Kinetics in Atmospheric Gases (Berlin: Springer) (2000).*
10. *Kossyi I A, Kostinsky A Yu, Matveyev A A and Silakov V P, Kinetic scheme on the non-equilibrium discharge in nitrogen–oxygen mixtures, Plasma Sources Sci. Technol.* ***1*** *207 (1992).*

11. *Yu Akishev, M Grushin, V Karalnik, A Petryakov and N Trushkin, " On basic processes sustaining constricted glow discharge in longitudinal N 2 flow at atmospheric pressure", J. Phys. D: Appl. Phys. 43 (2010) 215202 (18pp).*
12. *Chikalthankar, S. B., Nandedkar, V. M., & Borde, S. V. (2013). Influence of Machining Parameters on Electric Discharge Machining of WPS Tool Steels–An Experimental Investigation. International Journal of Mechanical and Production Engineering Research and Development (IJMPERD), 3(5), 21–28.*
13. *article.ajmp.org.*
14. *www. valmirmateus.blogspot.com.*
15. *K. A. Vereshchagin, V. V. Smirnov, V. A. Shakhatov, CARS study of the vibrational kinetics of nitrogen molecules in the burning and afterglow stages of a pulsed discharge, Moscow Radio Engineering Institute, Russian Academy of Sciences, 113519, (1995).*
16. *Job, V. M., & Gunakala, S. R. (2013). Unsteady MHD Free Convection Couette Flow between Two Vertical Permeable Plates in the Presence of Thermal Radiation Using Galerkin's Finite Element Method. International Journal of Mechanical Engineering, 2(5), 99-110.*